

## AB-INITIO CALCULATION OF REDOX POTENTIALS OF TITANIUM CATIONS IN SOLUTION

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Quantum-chemical calculation of inter-ion redox potentials for transition metal cations in water, with accuracy comparable to the experimental one, has not been possible until recently. We have developed the necessary methodology to calculate redox potentials between hydrated titanium cation solutions (charges +2, +3, +4).

The following components are included in the model:

- full geometry optimization of two coordination spheres (total of 18) of water molecules;
- zero-point energy corrections from vibrational analysis of the full complexes;
- continuum solvation effects using the COSMO model;
- volume change effects from general thermodynamics;
- relativistic correction to energy (literature value);
- entropy factor required for estimation of redox potentials was the only component derived from experimental data.

Both the  $\text{Ti}^{2+}/\text{Ti}^{3+}$  and  $\text{Ti}^{3+}/\text{Ti}^{4+}$  redox potentials were calculated within 0.1 V from the experimental values, which is the same accuracy as the that of the available experimental data.

Work is under way to check the model on other transition metal cations.

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